ON THE THEORY OF STARK BROADENING OF SPECTRAL LINES IN A PLASMA

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ABSTRACT

The theory of Stark broadening of isolated spectral lines by electrons in a plasma was developed by Griem et al (ref. 1), and numerical results were obtained for a large number of neutral and singly ionized spectral lines (ref. 2). Large discrepancies between measured and predicted widths of ion lines (e.g., Jalufka et al, ref. 3 and 4) have led to a reinvestigation of the underlying assumptions. It is shown that the calculated widths do not change by more than a few percent as a result of certain corrections. The effect of different strong collision cutoff procedures is as important but still far too small to explain the experimental results for ions. Debye shielding must often be taken into account in the electron density determinations from broadening of neutral lines in typical experiments and was therefore built into a computer program for electron impact widths. The results are compared with estimates on the basis of the usual procedure (ref. 1) for estimating Debye shielding effects.

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I. INTRODUCTION

A sizable discrepancy between experiment and theory in the Stark broadening of lines emitted by singly charged argon ions has been reported previously (refs. 3 and 4). The measured lines were wider by factors of typically 2.5.

The Stark broadening theory for isolated lines has been reviewed critically in an effort to determine the cause of this discrepancy. J. Cooper[1] and the author are cooperating in the development of a generalization of the relevant Stark broadening theory (ref. 1) which has succeeded in removing the discrepancy for all cases for which numerical results are now available (for a different approach see also ref. 5). While it would be premature to present details of this most recent development it is considered to be appropriate to report some refinements to the theory as published in reference 1 (GBKO).

II. THE STARK BROADENING FUNCTIONS

The functions $A(z)$ and $B(z)$ which arise from the first nonvanishing term in the Dyson series in GBKO are defined by

$$A(z) + iB(z) = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{x_1} dx_2 \, e^{iz(x_1-x_2)} \, f(x_1,x_2) \qquad (1)$$

[1]at JILA, Boulder, Colorado

with

$$f(x_1,x_2) = \frac{1}{2}\,\frac{1 + x_1x_2}{\left(1 + x_1^{\,2}\right)^{3/2}\left(1 + x_2^{\,2}\right)^{3/2}}$$

Width and shift due to electron impact broadening are proportional to thermal averages over the functions $a(z)$ and $b(z)$, respectively, which are defined by

$$\text{WIDTH} \sim \left[\int_z^\infty A(z)\,\frac{dz}{z}\right]_{th} = a(z)_{\;th} \tag{2}$$

$$\text{SHIFT} \sim \left[\int_z^\infty B(z)\,\frac{dz}{z}\right]_{th} = b(z)_{\;th} \tag{3}$$

While $A(z)$ had been expressed in terms of modified Bessel functions in GBKO the important function $a(z)$ had been obtained numerically on a digital computer. It turns out that the integral can be evaluated analytically, and that the resulting $a(z)$ is consistently smaller than used in GBKO:

$$a(z) = z\,K_0(|z|)\,K_1(|z|) \tag{4}$$

As in GBKO, K_0 and K_1 are modified Bessel functions. Figure 1 shows $a(z)$ along with its asymptotic forms for small and large z and with the numerical results of GBKO for comparison.

Since most of the broadening comes from $z \ll 1$ where the correct asymptotic form was used in GBKO one would expect little effect on the numbers computed there and in later reports by Griem. This is illustrated by table 1 which shows some widths computed with the old and new functions. The change of about five percent or less is probably negligible compared to the uncertainties in the matrix elements. It may also be noted that a comparable uncertainty is introduced by the choice of the strong collision cutoff.

TABLE 1

WIDTHS [Å] AT 10^{16} ELECTRONS/CM^3

	a(z) From:	GBKO[1]	Present Form
HE 5876	Cutoff I (see footnote 2)	$.17_3$	$.16_4$
	" II (see footnote 3)	$.18_3$	$.17_4$
HE 5016	" I	$.36_0$	$.34_8$
	" II	$.37_7$	$.36_5$
AR II 4806	" I	$.010_0$	$.009_5$
	" II	$.012_2$	$.011_6$

The function B(z) is obtained numerically via the principal value integral

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[1] as recalculated by this author.

[2] as in reference 1.

[3] as in reference 2.

$$B(z) = \frac{2z}{\pi} \text{ P.V.} \int_{0}^{\infty} \frac{A(z')}{z^2 - z'^2} \, dz' \tag{5}$$

Revised values of $B(z)$ between $0 \leq z \leq 5$ are within typically one percent of those in GBKO. However, $b(z)$ had to be increased by nearly 20 percent for small values of z. This is illustrated in figure 2 where $B(z)$ and $b(z)$ are plotted along with $b(z)$ as given in GBKO.

Unlike the values in GBKO the revised values were obtained by integrating over $\frac{B(z)}{2}$ from z to infinity. An excellent check is provided by the known value $b(o) = \frac{\pi}{2}$ (GBKO). The revised value is equal to $\pi/2$ within better than one percent although (see eq. 3) the integration over $B(z)/z$ must be carried out over the entire range of z (0 to ∞) to obtain $b(o)$. Although the new values differ most from the GBKO values for $z < 2$, the resulting changes by typically 10 percent in the shift are not critical because of the inherently much larger uncertainties in all computed shifts.

The successful redetermination of $b(z)$ was made possible by a much extended asymptotic expansion of $B(z)$ and $b(z)$. It can be shown that the asymptotic expansions of $B(z)$ and $b(z)$ for large z are

$$B(z) = \sum_{n=1}^{k} \frac{a_n}{z^{2n-1}} \tag{6}$$

and

$$b(z) = \sum_{n=1}^{k} \frac{a_n}{(2n - 1)z^{2n-1}} \tag{7}$$

respectively, with

$$a_n = \int_{-\infty}^{\infty} \left[\frac{d^{2n-2} f\ x_1, x_2}{dx_2^{\ 2n-2}} \right]_{x_2 - x_1} \tag{8}$$

$f\left(x_1, x_2\right)$ is the same as in equation 1.

It can now be shown with a considerable amount of algebra that

$$\begin{aligned} a_n = \frac{\pi}{2} \Bigg\{ & \prod_{i=1}^{\frac{n-1}{2}} (2i+1) \sum_{i=1}^{\frac{n+1}{2}} \Bigg[\binom{\frac{n-1}{2}}{i-1} (-1)^{i-1} \prod_{j=1}^{n-i+2} \left(1 - \frac{1}{2j}\right) \\ & \times \prod_{j=1}^{\frac{n+1}{2}-i} (n+2j) \prod_{j=1}^{i-1} (n+3-2j) \Bigg] - \prod_{i=1}^{\frac{n+1}{2}} (2i-1)(-1)^i \sum_{i=1}^{\frac{n+1}{2}} \binom{\frac{n-1}{2}}{i-1} \\ & \times \prod_{j=1}^{\frac{n+1}{2}-i} (n+2j) \prod_{j=1}^{i-1} (n+1-2j) \left[\prod_{j=1}^{n+1-i} \left(1 - \frac{1}{2j}\right) - \prod_{j=1}^{n+2-i} \left(1 - \frac{1}{2j}\right) \right] \Bigg\} \end{aligned} \tag{9}$$

This expression is best evaluated on a computer. The first few coefficients are listed in table 2.

TABLE 2

COEFFICIENTS OF THE ASYMPTOTIC EXPANSION OF $B(z)$

n	a_n
1	$\pi/4 = .7854$
3	$9\pi/32 = .8836$
5	4.142
7	42.28
9	750.4

At $z = 5$ the asymptotic value for $B(z)$ to order z^{-9} agrees with the revised value from the principle value integration within .02 percent.

III. DEBYE SHIELDING

Debye shielding is often only a correction and may be taken into account approximately by the procedure outlined by GBKO. A shielded width w_s may be estimated from the tabulated unshielded width w_o by

$$w_s \approx w_o \left(1 - \frac{a\left(\frac{\omega_{\alpha\alpha'}}{\omega_p}\right)}{a\left(\frac{\rho_{min}\,\omega_{\alpha\alpha'}}{\bar{v}}\right)} \right) \tag{10}$$

where $\omega_{\alpha\alpha'}$ is the separation (in angular frequency units) of the closest perturbing level, ω_p the plasma frequency, $\bar{v}$ the mean thermal electron speed, and ρ_{min} the minimum impact parameter. Since $a\left(z_{\alpha\alpha'}^{min}\right)$ should be reduced by $a\left(z_{\alpha\alpha'}^{max}\right)$, which means that the integration over impact parameters ρ is cut off at the Debye length ρ_D rather than extended to ∞, the ratio on the right side should estimate the effect if a typical v and the most important level α' are used.

This procedure overestimates the reduction of the width not only because it neglects the other perturbing levels α', but also because the width vanishes even for a single level α' as soon as ρ_{max} approaches ρ_{min} at $v = \bar{v}$. However, for $v > \bar{v}$, ρ_{min} is smaller than at $v = \bar{v}$, so that a finite contribution to the width remains. If Debye shielding is important, that is, if the plasma frequency becomes of the order of the level spacing $\omega_{\alpha\alpha'}$ between the initial (or final) state and the perturbing level α', the effect of Debye shielding should be subtracted from the contribution of each perturbing level separately, and before the thermal average is taken:

$$w_s \sim \left\langle \sum_{\alpha'} \left[a\left(z_{\alpha\alpha'}^{min}\right) - a\left(z_{\alpha\alpha'}^{max}\right) \right] \right\rangle_{th} \tag{11}$$

A comparison has been made between w_s according to equations (10) and (11) for the He I 5876 line. Figure 3 shows the ratios w/N_e and s/w versus electron density. The estimated ratio w/N_e is also shown and can be seen to be reliable for width reductions of about 25 percent in this instance. The shift is considerably more sensitive to Debye shielding. In particular, Debye shielding must be considered if the first order independence of the shift/width ratio is to be utilized for electron temperature determinations, even if this plasma thermometer, first suggested by D. D. Burgess (ref. 6), is calibrated experimentally.

The measurements of argon II broadening (refs. 3 and 4) were carried out at 10^{17} electrons/cm^3 density where Debye shielding is negligible for the He 5876 line which served for the density determination.

IV. SUMMARY

In summary, the facts reported today are refinements to the mathematics involved in the GBKO theory and point to a need for line broadening calculations which include Debye shielding. Such calculations are in progress at Langley. It is also concluded that the GBKO theory in its present form does fail for isolated lines of singly charged ions. The development of a more satisfactory theory is in progress.

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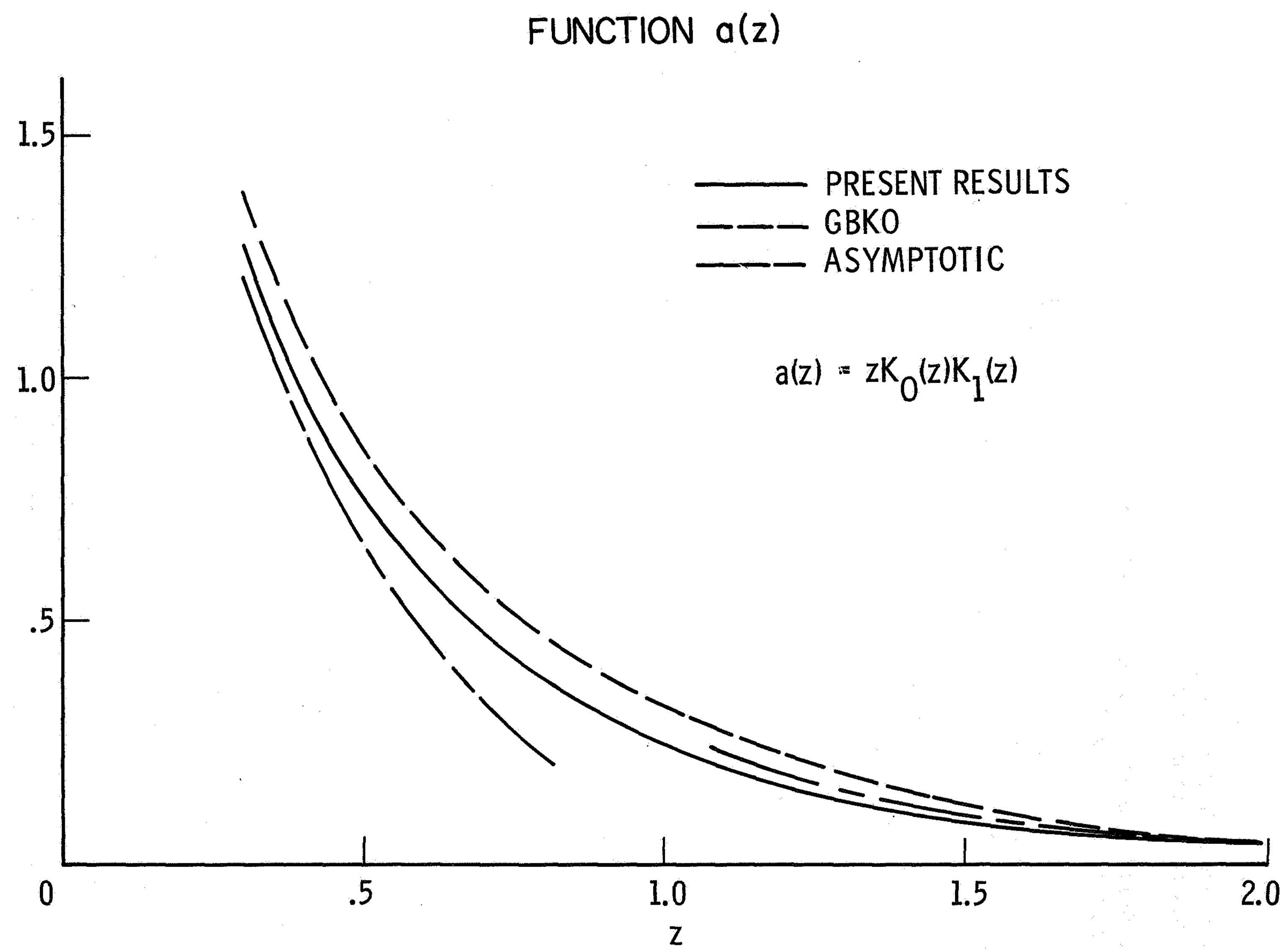
FUNCTION a(z)
PRESENT RESULTS
GBKO
ASYMPTOTIC
a(z) = zK0(z)K1(z)
1.5
1.0
.5
0
.5
1.0
1.5
2.0
z

Figure 1

FUNCTIONS B(z), b(z)

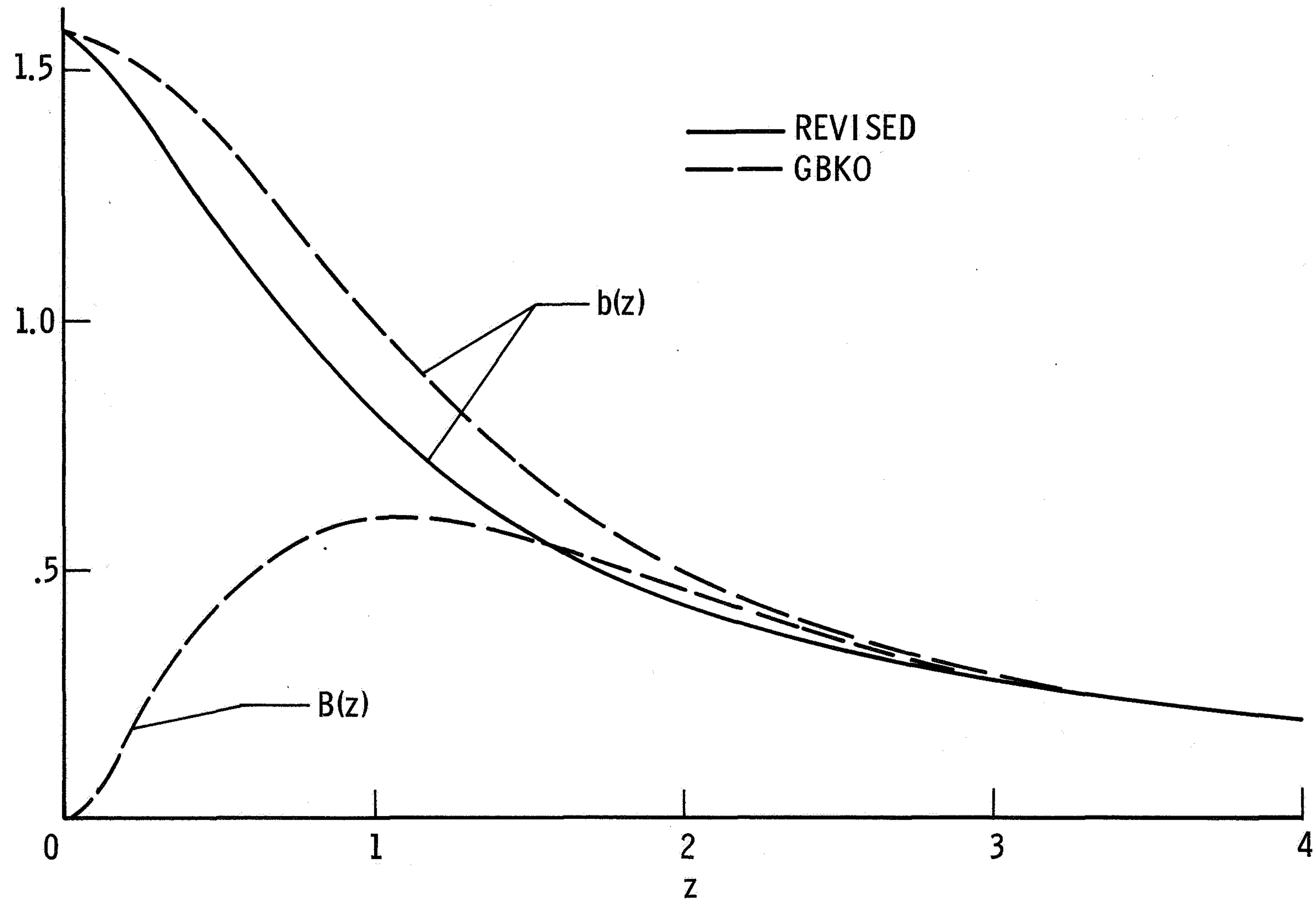

Figure 2

DEBYE SHIELDING, HE 5876 Å

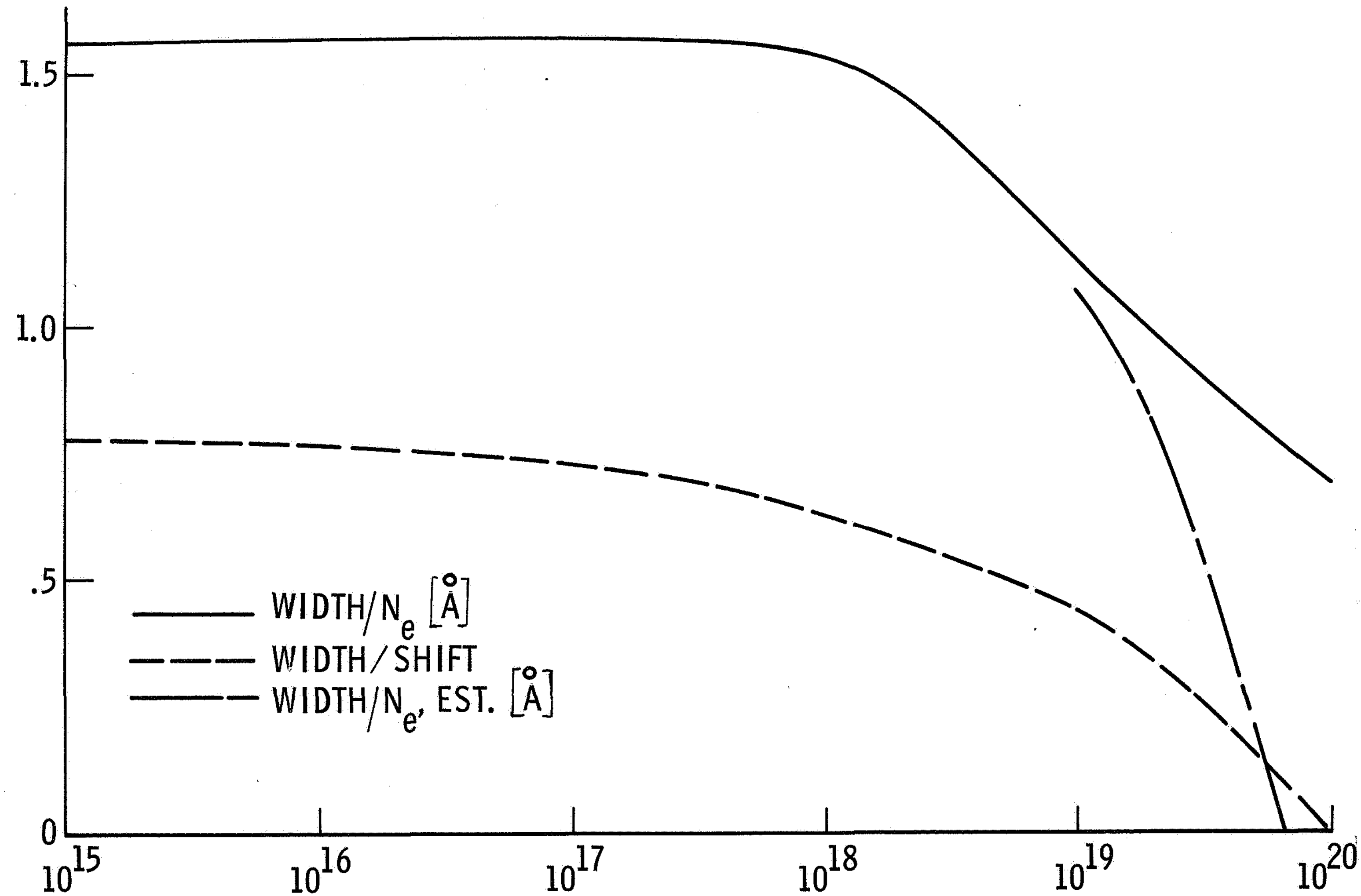

Figure 3

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